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RESEARCH AND DEVELOPMENT TECHNICAL REPORT
SLCET-TR-89-2

AD-A208 349

POLARIZATION MATRICES OF LITHIUM TANTALATE

ARTHUR BALLATO
ELECTRONICS TECHNOLOGY AND DEVICES LABORATORY

APRIL 1989

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SECURITY CLASSIFICATION OF THIS PAGE

REPORT DOCUMENTATION PAGE

Form Approved
OMB No. 0704-0188

| | | | | | |
|--|-------|--|---|---|----------------------------------|
| 1a. REPORT SECURITY CLASSIFICATION Unclassified | | | 1b. RESTRICTIVE MARKINGS | | |
| 2a. SECURITY CLASSIFICATION AUTHORITY | | | 3. DISTRIBUTION/AVAILABILITY OF REPORT Approved for public release; distribution is unlimited. | | |
| 2b. DECLASSIFICATION/DOWNGRADING SCHEDULE | | | | | |
| 4. PERFORMING ORGANIZATION REPORT NUMBER(S) SLCET-TR-89-2 | | | 5. MONITORING ORGANIZATION REPORT NUMBER(S) | | |
| 6a. NAME OF PERFORMING ORGANIZATION US Army Laboratory Command Electronics Tech & Devices Lab | | 6b. OFFICE SYMBOL (If applicable) SLCET-MA-A | | 7a. NAME OF MONITORING ORGANIZATION | |
| 6c. ADDRESS (City, State, and ZIP Code) Electronics Technology and Devices Laboratory ATTN: SLCET-MA-A Fort Monmouth, NJ 07703-5000 | | | | 7b. ADDRESS (City, State, and ZIP Code) | |
| 8a. NAME OF FUNDING/SPONSORING ORGANIZATION | | 8b. OFFICE SYMBOL (If applicable) | | 9. PROCUREMENT INSTRUMENT IDENTIFICATION NUMBER | |
| 8c. ADDRESS (City, State, and ZIP Code) | | | | 10. SOURCE OF FUNDING NUMBERS | |
| | | PROGRAM ELEMENT NO. 1L162705- | | PROJECT NO. H94 | TASK NO. K9 |
| | | | | WORK UNIT ACCESSION NO. DA303394 | |
| 11. TITLE (Include Security Classification) POLARIZATION MATRICES OF LITHIUM TANTALATE (U) | | | | | |
| 12. PERSONAL AUTHOR(S) Arthur Ballato | | | | | |
| 13a. TYPE OF REPORT Technical Report | | 13b. TIME COVERED FROM Jan 88 to Jan 89 | | 14. DATE OF REPORT (Year, Month, Day) 1989 April | |
| 15. PAGE COUNT 27 | | | | | |
| 16. SUPPLEMENTARY NOTATION | | | | | |
| 17. COSATI CODES | | | 18. SUBJECT TERMS (Continue on reverse if necessary and identify by block number) | | |
| FIELD | GROUP | SUB-GROUP | | | |
| 09 | 01 | | Piezoelectric resonators; piezoelectric transducers; | | |
| 17 | 02 | | lithium tantalate; acousto-optics, tantalum compounds, lithium compounds, (lithium) | | |
| 19. ABSTRACT (Continue on reverse if necessary and identify by block number) | | | | | |
| <p>In analytical treatments of piezoelectric/acoustic transducers, signal processors, and resonators, the electromechanical transduction mechanism is most often expressed in terms of the elements of the piezoelectric [e] or [d] matrices. Molecular interpretations of piezoelectricity, and especially electro-optical applications, usually involve polarization as the preferred variable, and consequently the alternative [a] and [b] matrices are of interest. The elements of these latter sets are calculated for lithium tantalate from measured elastopiezodielectric constants taken from the literature.</p> | | | | | |
| 20. DISTRIBUTION/AVAILABILITY OF ABSTRACT <input type="checkbox"/> UNCLASSIFIED/UNLIMITED <input checked="" type="checkbox"/> SAME AS RPT <input type="checkbox"/> DTIC USERS | | | 21. ABSTRACT SECURITY CLASSIFICATION Unclassified | | |
| 22a. NAME OF RESPONSIBLE INDIVIDUAL Dr. Arthur Ballato | | | 22b. TELEPHONE (Include Area Code) (201) 544-2773 | | 22c. OFFICE SYMBOL SLCET-MA A |

DD Form 1473, JUN 86

Previous editions are obsolete

SECURITY CLASSIFICATION OF THIS PAGE

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INTRODUCTION

Electromechanical transduction taking place via the piezoelectric effect is characterized phenomenologically by constitutive equations that relate the elastic and electric variables. These equations take a variety of forms, depending upon the choice of independent and dependent variables; the choice is normally dictated by the application. For example, piezoelectric resonators in the form of thickness mode plates are most easily treated using the isagrig elastic stiffnesses $[cE]$, the piezoelectric stress constants $[e]$, and the dielectric permittivities at constant strain $[(\epsilon_s)S]$.

Various measurement techniques yield values for the elements of a particular coefficient set more directly than those of another. The coefficients appearing in the different equation sets are, however, interrelated, so that once any one complete set is available, all the other sets of elements may be found. The most accurate and precise experimental results to date have been from plate resonator (resonance) and pulse-echo (transit-time) measurements. From the $[cE]$, $[e]$, and $[(\epsilon_s)S]$ matrices determined therefrom, those matrices representing material properties expressed in the other alternative forms may be calculated.

Electrooptical applications are becoming increasingly important. So also are treatments of piezoelectric and ferroelectric phenomena from the standpoint of molecular interactions. In both of these cases the constitutive equations using polarization as the independent electrical variable, rather than either electric intensity or displacement, assume greater importance than the sets traditionally used for transducer, signal processing, and resonator applications.

In this report we give the complete sets of linear constitutive equations relating elastic and electric fields. For each equation set the numerical values are computed for lithium tantalate, a highly piezoelectric ferroelectric with temperature-compensated orientations, from the measured $[cE]$, $[e]$, and $[(\epsilon_s)S]$ values of Smith and Welsh (Ref. 1). Coupling to the thermal field is neglected. Rationalized mks units are used throughout.

CONSTITUTIVE EQUATION SETS

Symbols and units for the quantities employed are given in Table 1. In terms of these, six constitutive equation sets are used. Of these, electric intensity, dielectric displacement, and polarization each appear in two sets as an independent variable. The sets are, in compressed matrix notation, as follows. A prime denotes transpose; $[I]$ is the unit matrix.

I. The Piezoelectric Stress Constant Set

$$\begin{aligned} [T] &= [cE] [S] - [e]' [E] & (1) \\ [D] &= [e] [S] + [(\epsilon_s)S] [E] & (2) \end{aligned}$$

TABLE 1. SYMBOLS, UNITS, AND DEFINITIONS.

| QUANTITY | UNIT | SYMBOL/DEFINITION |
|--|-------------------|---|
| Elastic stress | N/m ² | [T] |
| Elastic strain | ----- | [S] |
| Electric intensity | V/m | [E] |
| Dielectric displacement | C/m ² | [D] |
| Dielectric polarization | C/m ² | [P] |
| Elastic compliance at constant [E], [D], [P] | m ² /N | [cE], [cD], [cP] |
| Elastic stiffness at constant [E], [D], [P] | N/m ² | [sE], [sD], [sP] |
| Dielectric permittivity at constant [T], [S] | F/m | [(eps)T], [(eps)S] |
| Dielectric constant, relative, at constant [T], [S] | ----- | [(Kr)T], [(Kr)S] =[(eps)T]/(eps)o, [(eps)S]/(eps)o |
| Dielectric impermeability at constant [T], [S] | m/F | [(bet)T], [(bet)S] =[(eps)T] ⁽⁻¹⁾ , [(eps)S] ⁽⁻¹⁾ |
| Dielectric impermeability, relative, at constant [T], [S] | ----- | [(betr)T], [(betr)S] =[(bet)T]*(eps)o, [(bet)S]*(eps)o =[(Kr)T] ⁽⁻¹⁾ , [(Kr)S] ⁽⁻¹⁾ |
| Dielectric susceptibility at constant [T], [S] | F/m | [(chi)T], [(chi)S] =[(Kr)T-I]*(eps)o, [(Kr)S-I]*(eps)o |
| Dielectric susceptibility, relative, at constant [T], [S] | ----- | [(chir)T], [(chir)S] =[(chi)T]/(eps)o, [(chi)S]/(eps)o |
| Reciprocal dielectric susceptibility at constant [T], [S] | m/F | [(zet)T], [(zet)S] =[(chi)T] ⁽⁻¹⁾ , [(chi)S] ⁽⁻¹⁾ |
| Reciprocal dielectric susceptibility, relative, at constant [T], [S] | ----- | [(zetr)T], [(zetr)S] =[(zet)T]*(eps)o, [(zet)S]*(eps)o |
| Piezoelectric stress constant | C/m ² | [e] |

TABLE 1. SYMBOLS, UNITS, AND DEFINITIONS. (continued)

| QUANTITY | UNIT | SYMBOL/DEFINITION |
|-------------------------------------|-------------|-------------------|
| Piezoelectric strain coefficient | $m/V = C/N$ | [d] |
| Piezoelectric stress modulus | $N/C = V/m$ | [h] |
| Piezoelectric strain constant | m^2/C | [g] |
| Piezoelectric polarization modulus | $V/m = N/C$ | [a] |
| Piezoelectric polarization constant | m^2/C | [b] |

Note: Square brackets, sic: [], denote matrices.

II. The Piezoelectric Strain Coefficient Set

$$\begin{aligned} [S] &= [sE] [T] + [d]' [E] & (3) \\ [D] &= [d] [T] + [(\epsilon)sT] [E] & (4) \end{aligned}$$

III. The Piezoelectric Stress Modulus Set

$$\begin{aligned} [T] &= [cD] [S] - [h]' [D] & (5) \\ [E] &= -[h] [S] + [(\beta)sS] [D] & (6) \end{aligned}$$

IV. The Piezoelectric Strain Constant Set

$$\begin{aligned} [S] &= [sD] [T] + [g]' [D] & (7) \\ [E] &= -[g] [T] + [(\beta)sT] [D] & (8) \end{aligned}$$

V. The Piezoelectric Polarization Modulus Set

$$\begin{aligned} [T] &= [cP] [S] - [a]' [P] & (9) \\ [E] &= -[a] [S] + [(\zeta)sS] [P] & (10) \end{aligned}$$

VI. The Piezoelectric Polarization Constant Set

$$\begin{aligned} [S] &= [sP] [T] + [b]' [P] & (11) \\ [E] &= -[b] [T] + [(\zeta)sT] [P] & (12) \end{aligned}$$

The electric variables are connected by the relation

$$[D] = (\epsilon)s_o * [E] + [P] \quad (13)$$

where $(\epsilon)s_o$ is the permittivity of free space, defined by

$$(\epsilon)s_o * (\mu)o * (c) * (c) = 1 ; \quad (14)$$

$(\mu)o$ is the permeability of free space, equal, by definition, to $4 \pi * 10^{(-7)}$, and (c) is the velocity of light in vacuo and, also by definition, is equal exactly to 2.99792458×10^8 m/s.

From (13) the expressions for the remaining electric variables associated, respectively, with the six equation sets (1) to (12) may be found:

$$[P] = [e] [S] + [(\chi)sS] [E] \quad (15)$$

$$[P] = [d] [T] + [(\chi)sT] [E] \quad (16)$$

$$[P] = (\epsilon)s_o * [h] [S] + [1 - (\epsilon)s_o * (\beta)sS] [D] \quad (17)$$

$$[P] = (\epsilon)s_o * [g] [T] + [1 - (\epsilon)s_o * (\beta)sT] [D] \quad (18)$$

$$[D] = -(\epsilon)_o * [a] [S] + [I + (\epsilon)_o * (\zeta)S] [P] \quad (19)$$

$$[D] = -(\epsilon)_o * [b] [T] + [I + (\epsilon)_o * (\zeta)T] [P] \quad (20)$$

RELATIONS AMONG MATERIAL CONSTANTS

The material constants are interrelated by the following formulas:

$$[cX] [sX] = [(\epsilon)Y] [(\beta)Y] = [I] \quad (21)$$

$$[(\chi)Y] [(\zeta)Y] = [(Kr)Y - (\chi)Y] = [I] \quad (22)$$

In (21) and (22), X = E, D, or P and Y = T or S.

$$\begin{aligned} [cD] - [cE] &= [h]' [e] = [e]' [h] \\ &= [h]' [(\epsilon)S] [h] = [e]' [(\beta)S] [e] \\ &= [a]' [e - h * (\epsilon)_o] = [e - h * (\epsilon)_o]' [a] \end{aligned} \quad (23)$$

$$\begin{aligned} [cP] - [cD] &= [h]' [a] * (\epsilon)_o = [a]' [h] * (\epsilon)_o \\ &= [h]' [(\epsilon)S] [(\zeta)S] [h] * (\epsilon)_o \\ &= [a]' [(\beta)S] [(\chi)S] [a] * (\epsilon)_o \\ &= [a - h]' [e] = [e]' [a - h] \end{aligned} \quad (24)$$

$$\begin{aligned} [cP] - [cE] &= [a]' [e] = [e]' [a] \\ &= [a]' [(\chi)S] [a] = [e]' [(\zeta)S] [e] \\ &= [h]' [e + a * (\epsilon)_o] = [e + a * (\epsilon)_o]' [h] \end{aligned} \quad (25)$$

$$\begin{aligned} [sE] - [sD] &= [d]' [g] = [g]' [d] \\ &= [d]' [(\beta)t] [d] = [g]' [(\epsilon)t] [g] \\ &= [b]' [d - g * (\epsilon)_o] = [d - g * (\epsilon)_o]' [b] \end{aligned} \quad (26)$$

$$\begin{aligned} [sD] - [sP] &= [b]' [g] * (\epsilon)_o = [g]' [b] * (\epsilon)_o \\ &= [g]' [(\epsilon)T] [(\zeta)T] [g] * (\epsilon)_o \\ &= [b]' [(\beta)T] [(\chi)T] [b] * (\epsilon)_o \\ &= [b - g]' [d] = [d]' [b - g] \end{aligned} \quad (27)$$

$$\begin{aligned} [sE] - [sP] &= [b]' [d] = [d]' [b] \\ &= [b]' [(\chi)T] [b] = [d]' [(\zeta)T] [d] \\ &= [g]' [d + b * (\epsilon)_o] = [d + b * (\epsilon)_o]' [g] \end{aligned} \quad (28)$$

$$\begin{aligned}
[(\text{zet})S] - [(\text{zet})T] &= [b] [a]' = [a] [b]' \\
&= [b] [cP] [b]' = [a] [sP] [a]' \quad (29)
\end{aligned}$$

$$\begin{aligned}
[(\text{chi})T] - [(\text{chi})S] &= [(\text{eps})T] - [(\text{eps})S] \\
&= [e] [d]' = [d] [e]' \\
&= [d] [cE] [d]' = [e] [sE] [e]' \quad (30)
\end{aligned}$$

$$\begin{aligned}
[(\text{bet})S] - [(\text{bet})T] &= [h] [g]' = [g] [h]' \\
&= [g] [cD] [g]' = [h] [sD] [h]' \quad (31)
\end{aligned}$$

$$[e] = [d] [cE] = [(\text{eps})S] [h] = [(\text{chi})S] [a] \quad (32)$$

$$[d] = [e] [sE] = [(\text{eps})T] [g] = [(\text{chi})T] [b] \quad (33)$$

$$\begin{aligned}
[h] = [g] [cD] &= [(\text{bet})S] [e] = [(\text{chi})S] [(\text{bet})S] [a] \\
&= [I - (\text{bet})S * (\text{eps})o] [a] \quad (34)
\end{aligned}$$

$$\begin{aligned}
[g] = [h] [sD] &= [(\text{bet})T] [d] = [(\text{chi})T] [(\text{bet})T] [b] \\
&= [I - (\text{bet})T * (\text{eps})o] [b] \quad (35)
\end{aligned}$$

$$\begin{aligned}
[a] = [b] [cP] &= [(\text{zet})S] [e] = [(\text{eps})S] [(\text{zet})S] [h] \\
&= [I + (\text{zet})S * (\text{eps})o] [h] \quad (36)
\end{aligned}$$

$$\begin{aligned}
[b] = [a] [sP] &= [(\text{zet})T] [d] = [(\text{eps})T] [(\text{zet})T] [g] \\
&= [I + (\text{zet})T * (\text{eps})o] [g] \quad (37)
\end{aligned}$$

Some alternative relations are the following:

$$\begin{aligned}
[a - h] &= [(\text{zet})S] [h] * (\text{eps})o \\
&= [(\text{bet})S] [a] * (\text{eps})o \quad (38)
\end{aligned}$$

$$\begin{aligned}
[b - g] &= [(\text{zet})T] [g] * (\text{eps})o \\
&= [(\text{bet})T] [b] * (\text{eps})o \quad (39)
\end{aligned}$$

$$[e + a * (\text{eps})o] = [(\text{eps})S] [a] \quad (40)$$

$$[d + b * (\text{eps})o] = [(\text{eps})T] [b] \quad (41)$$

$$[e - h * (\text{eps})o] = [(\text{chi})S] [h] \quad (42)$$

$$[d - g * (\text{eps})o] = [(\text{chi})T] [g] \quad (43)$$

Equations (21) to (43) result from equating like dependent variables in pairs selected from equations (1) to (12) and (15) to (20). Each

pair yields one equation in three variables, one mechanical and two electrical, or vice versa. Two other equations exist, again from (1) to (12) and (15) to (20), that contain the same three variables found in each paired equation. One of these auxiliary equations is used to eliminate one of the two variables of the same kind; the result is one equation in two variables, one electrical and one mechanical. These are now independent variables, so the coefficients must vanish; two relations between the material coefficients result. As an example, (3) and (7) both have [S] as dependent variable. Equating them produces one relation in [T], [E], and [D]; one of the electrical variables must be eliminated. This is done by using either (4) or (8); each contains the same three variables. If (8) is used to eliminate [E], one obtains $[sE - d'g - sD] [T] = [d'(\text{bet})T - g'] [D]$. Therefore, $[sE] - [sD] = [d]' [g]$ and $[g] = [(\text{bet})T] [d]$. Use of (4) instead of (8) leads to the equations $[sE] - [sD] = [g]' [d]$ and $[d] = [(\text{eps})T] [g]$. There are 36 pairs, six each equating [S] and [T], and eight each equating [E], [D], and [P]. The 72 relations contain many redundancies. Relations between the elastic, piezoelectric, and dielectric constants are shown schematically in Tables 2 and 3.

CALCULATION SEQUENCE

Using as input [cE], [e], and [(eps)S], one may compute the remaining quantities in a variety of ways. The following sequence is typical:

$$[sE] = [cE] \quad (-1) \quad (44)$$

$$[(\text{bet})S] = [(\text{eps})S] \quad (-1) \quad (45)$$

$$[d] = [e] [sE] \quad (46)$$

$$[h] = [(\text{bet})S] [e] \quad (47)$$

$$[(\text{eps})T] - [(\text{eps})S] = [e] [d]' \quad (48)$$

$$[(\text{eps})T] = [(\text{eps})S] + [e] [d]' \quad (49)$$

$$[(\text{bet})T] = [(\text{eps})T] \quad (-1) \quad (50)$$

$$[cD] - [cE] = [e]' [h] \quad (51)$$

$$[cD] = [cE] + [e]' [h] \quad (52)$$

$$[g] = [(\text{bet})T] [d] \quad (53)$$

$$[sE] - [sD] = [d]' [g] \quad (54)$$

$$[sD] = [sE] - [d]' [g] \quad (55)$$

$$[(\text{betr})S] = [(\text{bet})S] * (\text{eps})_0 \quad (56)$$

$$[(\text{zetr})S] = [(\text{betr})S] (I - (\text{betr})S) \quad (-1) \quad (57)$$

$$[(\text{zet})S] = [(\text{zetr})S] / (\text{eps})_0 \quad (58)$$

TABLE 2. RELATIONS AMONG MATERIAL CONSTANTS.

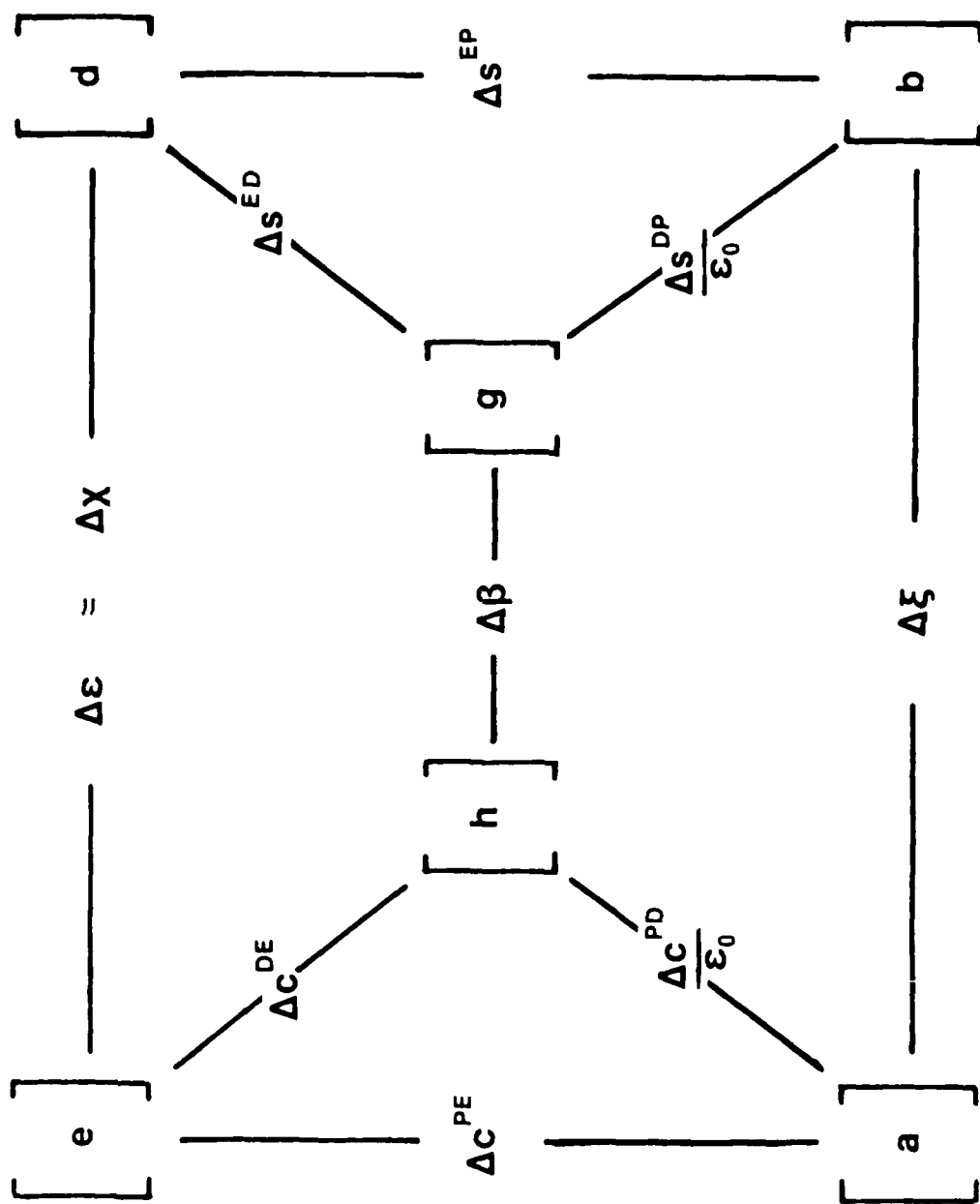
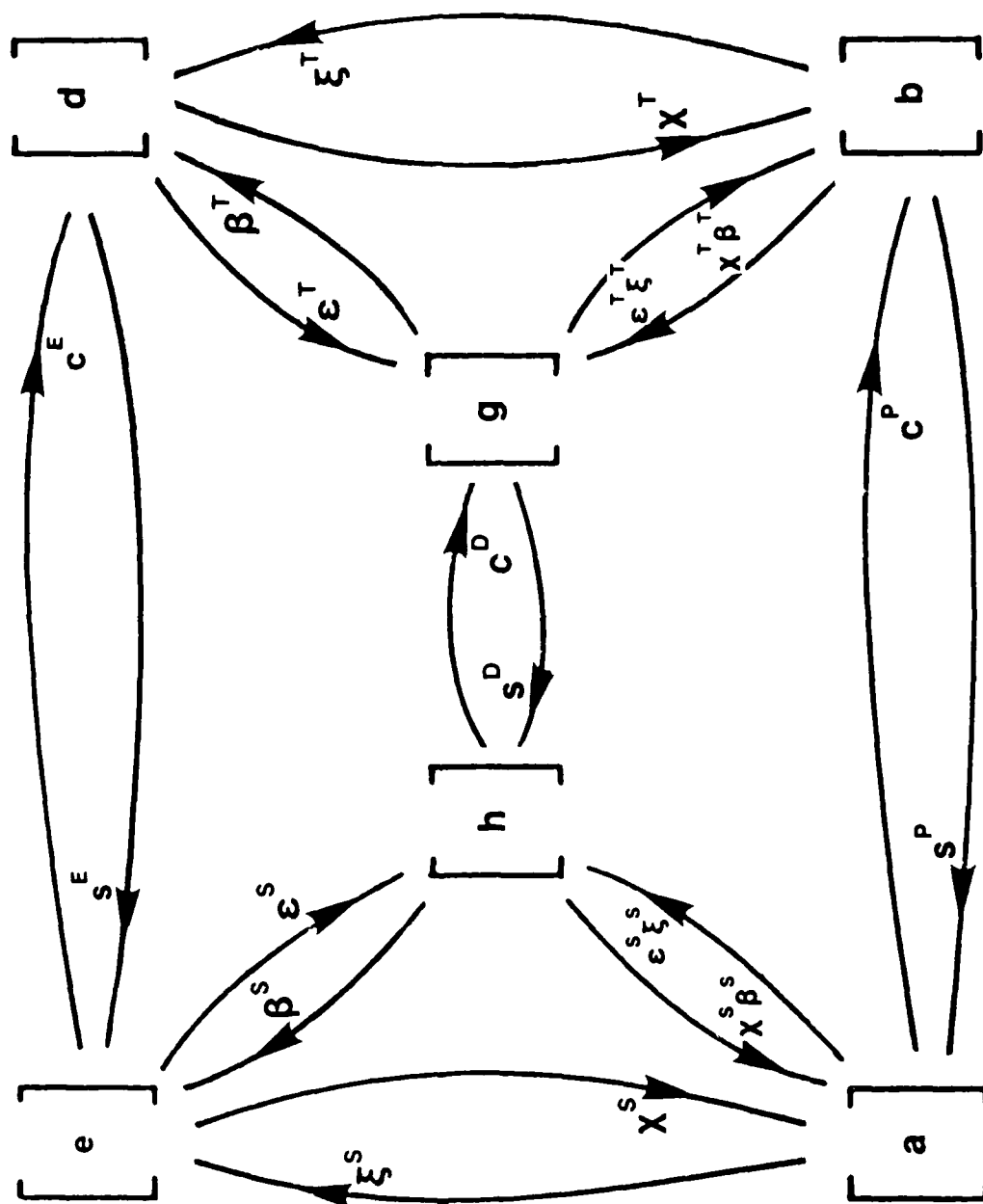


TABLE 3. FURTHER RELATIONS AMONG MATERIAL CONSTANTS.



$$[(\text{betr})T] = [(\text{bet})T] * (\text{eps})_o \quad (59)$$

$$[(\text{zetr})T] = [(\text{betr})T] [I - (\text{betr})T]^{(-1)} \quad (60)$$

$$[(\text{zet})T] = [(\text{zetr})T] / (\text{eps})_o \quad (61)$$

$$[(\text{chi})S] = [(\text{zet})S]^{(-1)} \quad (62)$$

$$[(\text{chi})T] = [(\text{zet})T]^{(-1)} \quad (63)$$

$$[a] = [(\text{zet})S] [e] \quad (64)$$

$$[b] = [(\text{zet})T] [d] \quad (65)$$

$$[cP] - [cE] = [e]' [a] \quad (66)$$

$$[cP] = [cE] + [e]' [a] \quad (67)$$

$$[cP] - [cD] = [a]' [h] * (\text{eps})_o \quad (68)$$

$$[sE] - [sP] = [d]' [b] \quad (69)$$

$$[sP] = [sE] - [d]' [b] \quad (70)$$

$$[sD] - [sP] = [g]' [b] * (\text{eps})_o \quad (71)$$

$$[(\text{bet})S] - [(\text{bet})T] = [h] [g]' \quad (72)$$

$$[(\text{chi})T] - [(\text{chi})S] = [(\text{eps})T] - [(\text{eps})S] \quad (73)$$

$$[(\text{zet})S] - [(\text{zet})T] = [a] [b]' \quad (74)$$

A number of these relations are used as checks. For example, $[(\text{bet})S]$ and $[(\text{bet})T]$ are known from (45) and (50), but the difference is recomputed in (72).

EXPLICIT FORMULAS FOR POINT GROUP 3m

Elastic:

The 6x6 elastic constant portions of Tables 4 and 5 partition into 4x4 and 2x2 submatrices. The 4x4 elastic stiffness and compliance submatrices are interrelated by formulas (75) to (93), taken from Cady (Ref. 2):

$$A = s_{33} * (s_{11} + s_{12}) - 2 * s_{13} * s_{13} \quad (75)$$

$$B = s_{44} * (s_{11} - s_{12}) - 2 * s_{14} * s_{14} \quad (76)$$

$$2 * c_{11} = s_{33} / A + s_{44} / B \quad (77)$$

$$2 * c_{12} = s_{33} / A - s_{44} / B \quad (78)$$

$$c_{13} = - s_{13} / A ; \quad c_{14} = - s_{14} / B \quad (79a), (79b) \quad (79)$$

TABLE 4. ELASTOPIEZODIELECTRIC MATRICES FOR POINT GROUP 3m:
THE [e], [h], AND [a] SETS.

| | | | | | | | | | | |
|-----|-----|----|-----|----|-----|---|-----|-----|----|-------------|
| 11 | 12 | 13 | 14 | 00 | 00 |] | 00 | -22 | 31 | |
| | | | | | |] | | | | cE] e' |
| 12 | 11 | 13 | -14 | 00 | 00 |] | 00 | 22 | 31 | -----]----- |
| | | | | | |] | | | | e] (eps)S |
| 13 | 13 | 33 | 00 | 00 | 00 |] | 00 | 00 | 33 | |
| | | | | | |] | | | | |
| 14 | -14 | 00 | 44 | 00 | 00 |] | 00 | 15 | 00 | cD] h' |
| | | | | | |] | | | | -----]----- |
| 00 | 00 | 00 | 00 | 44 | 14 |] | 15 | 00 | 00 | h] (bet)S |
| | | | | | |] | | | | |
| 00 | 00 | 00 | 00 | 14 | 66 |] | -22 | 00 | 00 | |
| | | | | | |] | | | | |
| 00 | 00 | 00 | 00 | 15 | -22 |] | 11 | 00 | 00 | |
| | | | | | |] | | | | cP] a' |
| -22 | 22 | 00 | 15 | 00 | 00 |] | 00 | 11 | 00 | -----]----- |
| | | | | | |] | | | | a] (zet)S |
| 31 | 31 | 33 | 00 | 00 | 00 |] | 00 | 00 | 33 | |

$$66 = (11 - 12) / 2$$

Matrix entries show only subscripts.

TABLE 5. ELASTOPIEZODIELECTRIC MATRICES FOR POINT GROUP 3m:
THE [d], [g], AND [b] SETS.

| | | | | | | | | | | |
|-----|-----|----|-----|------|-------|---|-------|-----|----|-------------|
| 11 | 12 | 13 | 14 | 00 | 00 |] | 00 | -22 | 31 | |
| | | | | | |] | | | | sE] d' |
| 12 | 11 | 13 | -14 | 00 | 00 |] | 00 | 22 | 31 | -----]----- |
| | | | | | |] | | | | d] (eps)T |
| 13 | 13 | 33 | 00 | 00 | 00 |] | 00 | 00 | 33 | |
| | | | | | |] | | | | |
| 14 | -14 | 00 | 44 | 00 | 00 |] | 00 | 15 | 00 | sD] g' |
| | | | | | |] | | | | -----]----- |
| 00 | 00 | 00 | 00 | 44 | 14*2 |] | 15 | 00 | 00 | g] (bet)T |
| | | | | | |] | | | | |
| 00 | 00 | 00 | 00 | 14*2 | 66 |] | -22*2 | 00 | 00 | |
| | | | | | |] | | | | |
| 00 | 00 | 00 | 00 | 15 | -22*2 |] | 11 | 00 | 00 | |
| | | | | | |] | | | | sP] b' |
| -22 | 22 | 00 | 15 | 00 | 00 |] | 00 | 11 | 00 | -----]----- |
| | | | | | |] | | | | b] (zet)T |
| 31 | 31 | 33 | 00 | 00 | 00 |] | 00 | 00 | 33 | |

$$66 = (11 - 12) * 2$$

Matrix elements show only subscripts.

$$c_{33} = (s_{11} + s_{12}) / A \quad (80)$$

$$c_{44} = (s_{11} - s_{12}) / B \quad (81)$$

$$c_{66} = (c_{11} - c_{12}) / 2 = s_{44} / (2 * B) \quad (82)$$

$$K = c_{33} * (c_{11} + c_{12}) - 2 * c_{13} * c_{13} \quad (83)$$

$$L = c_{44} * (c_{11} - c_{12}) - 2 * c_{14} * c_{14} \quad (84)$$

$$2 * s_{11} = c_{33} / K + c_{44} / L \quad (85)$$

$$2 * s_{12} = c_{33} / K - c_{44} / L \quad (86)$$

$$s_{13} = - c_{13} / K ; s_{14} = - c_{14} / L \quad (87a), (87b) \quad (87)$$

$$s_{33} = (c_{11} + c_{12}) / K \quad (88)$$

$$s_{44} = (c_{11} - c_{12}) / L \quad (89)$$

$$s_{66} = (s_{11} - s_{12}) = 2 * c_{44} / L \quad (90)$$

$$\det (4 \times 4) [s] = A * B \quad (91)$$

$$\det (4 \times 4) [c] = K * L \quad (92)$$

$$A * K = B * L = A * B * K * L = 1 \quad (93)$$

Formulas (75) to (93) hold for each set of constant electrical conditions: either E, D, or P constant.

$$[cD] - [cE] = [\text{del } cDE] = [e]' [h] = [h]' [e] \quad (23)$$

$$\text{del } cDE_{11} = + e_{22} h_{22} + e_{31} h_{31} \quad (94)$$

$$\text{del } cDE_{12} = - e_{22} h_{22} + e_{31} h_{31} \quad (95)$$

$$\text{del } cDE_{13} = + e_{31} h_{33} = + h_{31} e_{33} \quad (96)$$

$$\text{del } cDE_{14} = - e_{22} h_{15} = - h_{22} e_{15} \quad (97)$$

$$\text{del } cDE_{33} = + e_{33} h_{33} \quad (98)$$

$$\text{del } cDE_{44} = + e_{15} h_{15} \quad (99)$$

$$\text{del } cDE_{66} = + e_{22} h_{22} \quad (100)$$

$$\begin{aligned} [cP] - [cD] &= [\text{del } cPD] = [a]' [h] * (\text{eps})_0 \\ &= [h]' [a] * (\text{eps})_0 \end{aligned} \quad (24)$$

$$\text{del } cPD_{11} = (+ a_{22} h_{22} + a_{31} h_{31}) * (\text{eps})_0 \quad (101)$$

$$\text{del } cPD_{12} = (- a_{22} h_{22} + a_{31} h_{31}) * (\text{eps})_0 \quad (102)$$

$$\begin{aligned} \text{del cPD13} &= (+ a_{31} h_{33}) * (\text{eps})_o \\ &= (+ h_{31} a_{33}) * (\text{eps})_o \end{aligned} \quad (103)$$

$$\begin{aligned} \text{del cPD14} &= (- a_{22} h_{15}) * (\text{eps})_o \\ &= (- h_{22} a_{15}) * (\text{eps})_o \end{aligned} \quad (104)$$

$$\text{del cPD33} = (+ a_{33} h_{33}) * (\text{eps})_o \quad (105)$$

$$\text{del cPD44} = (+ a_{15} h_{15}) * (\text{eps})_o \quad (106)$$

$$\text{del cPD66} = (+ a_{22} h_{22}) * (\text{eps})_o \quad (107)$$

$$[cP] - [cE] = [\text{del cPE}] = [e]' [a] = [a]' [e] \quad (25)$$

$$\text{del cPE11} = + e_{22} a_{22} + e_{31} a_{31} \quad (108)$$

$$\text{del cPE12} = - e_{22} a_{22} + e_{31} a_{31} \quad (109)$$

$$\text{del cPE13} = + e_{31} a_{33} = + a_{31} e_{33} \quad (110)$$

$$\text{del cPE14} = - e_{22} a_{15} = - a_{22} e_{15} \quad (111)$$

$$\text{del cPE33} = + e_{33} a_{33} \quad (112)$$

$$\text{del cPE44} = + e_{15} a_{15} \quad (113)$$

$$\text{del cPE66} = + e_{22} a_{22} \quad (114)$$

From the del c13 entries we have the ratios

$$e_{31} / e_{33} = h_{31} / h_{33} = a_{31} / a_{33}. \quad (115)$$

From the del c14 entries we have the further ratios

$$e_{15} / e_{22} = h_{15} / h_{22} = a_{15} / a_{22}. \quad (116)$$

$$[sE] - [sD] = [\text{del sED}] = [d]' [g] = [g]' [d] \quad (26)$$

$$\text{del sED11} = + d_{22} g_{22} + d_{31} g_{31} \quad (117)$$

$$\text{del sED12} = - d_{22} g_{22} + d_{31} g_{31} \quad (118)$$

$$\text{del sED13} = + d_{31} g_{33} = + g_{31} d_{33} \quad (119)$$

$$\text{del sED14} = - d_{22} g_{15} = - g_{22} d_{15} \quad (120)$$

$$\text{del sED33} = + d_{33} g_{33} \quad (121)$$

$$\text{del sED44} = + d_{15} g_{15} \quad (122)$$

$$\text{del sED66} = + d_{22} g_{22} * 4 \quad (123)$$

$$[sD] - [sP] = [g]' [b] * (\epsilon s)o$$

$$= [b]' [g] * (\epsilon s)o \quad (27)$$

$$\text{del } sDP11 = (+ g22 b22 + g31 b31) * (\epsilon s)o \quad (124)$$

$$\text{del } sDP12 = (- g22 b22 + g31 b31) * (\epsilon s)o \quad (125)$$

$$\text{del } sDP13 = (+ g31 b33) * (\epsilon s)o$$

$$= (+ b31 g33) * (\epsilon s)o \quad (126)$$

$$\text{del } sDP14 = (- g22 b15) * (\epsilon s)o$$

$$= (- b22 g15) * (\epsilon s)o \quad (127)$$

$$\text{del } sDP33 = (+ g33 b33) * (\epsilon s)o \quad (128)$$

$$\text{del } sDP44 = (+ g15 b15) * (\epsilon s)o \quad (129)$$

$$\text{del } sDP66 = (+ g22 b22) * 4 * (\epsilon s)o \quad (130)$$

$$[sE] - [sP] = [\text{del } sEP] = [b]' [d] = [d]' [b] \quad (28)$$

$$\text{del } sEP11 = + d22 b22 + d31 b31 \quad (131)$$

$$\text{del } sEP12 = - d22 b22 + d31 b31 \quad (132)$$

$$\text{del } sEP13 = + d31 b33 = + b31 d33 \quad (133)$$

$$\text{del } sEP14 = - d22 b15 = - b22 d15 \quad (134)$$

$$\text{del } sEP33 = + d33 b33 \quad (135)$$

$$\text{del } sEP44 = + d15 b15 \quad (136)$$

$$\text{del } sEP66 = + d22 b22 * 4 \quad (137)$$

From the del s13 entries we have the ratios

$$d31 / d33 = g31 / g33 = b31 / b33. \quad (138)$$

From the del s14 entries we have the further ratios

$$d15 / d22 = g15 / g22 = b15 / b22. \quad (139)$$

Piezoelectric:

$$[d] = [e] [sE] \quad (33)$$

$$d15 = + e15 sE44 - e22 sE14 * 2 \quad (140)$$

$$d22 = + e22 (sE11 - sE12) - e15 sE14 \quad (141)$$

$$d_{31} = + e_{31} (s_{E11} + s_{E12}) + e_{33} s_{E13} \quad (142)$$

$$d_{33} = + e_{33} s_{E33} + e_{13} s_{E13} * 2 \quad (143)$$

$$[h] = [(bet)S] [e] \quad (34)$$

$$h_{15} = (bet)S_{11} e_{15} \quad (144)$$

$$h_{22} = (bet)S_{11} e_{22} \quad (145)$$

$$h_{31} = (bet)S_{33} e_{31} \quad (146)$$

$$h_{33} = (bet)S_{33} e_{33} \quad (147)$$

$$[g] = [(bet)T] [d] \quad (35)$$

$$g_{15} = (bet)T_{11} d_{15} \quad (148)$$

$$g_{22} = (bet)T_{11} d_{22} \quad (149)$$

$$g_{31} = (bet)T_{33} d_{31} \quad (150)$$

$$g_{33} = (bet)T_{33} d_{33} \quad (151)$$

$$[a] = [(zet)S] [e] \quad (36)$$

$$a_{15} = (zet)S_{11} e_{15} \quad (152)$$

$$a_{22} = (zet)S_{11} e_{22} \quad (153)$$

$$a_{31} = (zet)S_{33} e_{31} \quad (154)$$

$$a_{33} = (zet)S_{33} e_{31} \quad (155)$$

$$[b] = [(zet)T] [d] \quad (37)$$

$$b_{15} = (zet)T_{11} d_{15} \quad (156)$$

$$b_{22} = (zet)T_{11} d_{22} \quad (157)$$

$$b_{31} = (zet)T_{33} d_{31} \quad (158)$$

$$b_{33} = (zet)T_{33} d_{33} \quad (159)$$

Dielectric:

$$[(bet)Y] = [(eps)Y]^{(-1)} \quad (21)$$

$$(bet)Y_{11} = 1 / (eps)Y_{11} \quad (160)$$

$$(bet)Y_{33} = 1 / (eps)Y_{33} \quad (161)$$

$$[(\text{zetr})Y] = [(\text{betr})Y] [I - (\text{betr})Y]^{-1} \quad (162)$$

$$(\text{zet})Y_{11} = 1 / ((\text{eps})Y_{11} - (\text{eps})_0) \quad (163)$$

$$(\text{zet})Y_{33} = 1 / ((\text{eps})Y_{33} - (\text{eps})_0) \quad (164)$$

$$[(\text{eps})T - (\text{eps})S] = [\text{del } (\text{eps})] = [e] [d]' =$$

$$[(\text{chi})T - (\text{chi})S] = [\text{del } (\text{chi})] = [d] [e]' \quad (30)$$

$$\text{del } (\text{eps})_{11} = \text{del } (\text{chi})_{11} = + e_{15} d_{15} + e_{22} d_{22} * 2 \quad (165)$$

$$\text{del } (\text{eps})_{33} = \text{del } (\text{chi})_{33} = + e_{33} d_{33} + e_{31} d_{31} * 2 \quad (166)$$

$$[(\text{bet})S - (\text{bet})T] = [h] [g]' = [g] [h]' \quad (31)$$

$$\text{del } (\text{bet})_{11} = + h_{15} g_{15} + h_{22} g_{22} * 2 \quad (167)$$

$$\text{del } (\text{bet})_{33} = + h_{33} g_{33} + h_{31} g_{31} * 2 \quad (168)$$

$$[(\text{zet})S - (\text{zet})T] = [\text{del } (\text{zet})] = [a] [b]' = [b] [a]' \quad (169)$$

$$\text{del } (\text{zet})_{11} = + a_{15} b_{15} + a_{22} b_{22} * 2 \quad (170)$$

$$\text{del } (\text{zet})_{33} = + a_{33} b_{33} + a_{31} b_{31} * 2 \quad (171)$$

INPUT VALUES FOR LI TA 03

The values measured by Smith and Welsh (Ref.1) using the pulse-echo (transit-time) technique are as follows:

TABLE 6. ISAGRIC ELASTIC STIFFNESSES.

| cE11 | cE12 | cE13 | cE14 | cE33 | cE44 | cE66 |
|-------|------|------|-------|-------|------|------|
| 229.8 | 44.0 | 81.2 | -10.4 | 279.8 | 96.8 | 92.9 |

Units: 10^9 N/m².

TABLE 7. PIEZOELECTRIC STRESS CONSTANTS.

| e15 | e22 | e31 | e33 |
|------|------|-------|------|
| 2.72 | 1.67 | -0.38 | 1.09 |

Units: C/m².

TABLE 8. DIELECTRIC PERMITTIVITIES AT CONSTANT STRAIN.

| (eps)S11 | (eps)S33 |
|----------|----------|
| 377. | 379. |

Units: 10^{-12} F/m.

OUTPUT VALUES FOR LI TA 03

The input values from Tables 6, 7, and 8 were used to compute the remaining elastic, piezoelectric, and dielectric quantities for lithium tantalate in the manner discussed in prior sections of this report. The results are given in Tables 9 to 16.

TABLE 9. ELASTIC STIFFNESSES.

| | cE | cD | cP | del cDE | del cPE | del cPD |
|----|-------|-------|-------|---------|---------|---------|
| 11 | 229.8 | 237.6 | 237.8 | 7.78 | 7.976 | 0.187 |
| 12 | 44.0 | 37.0 | 36.8 | -7.02 | -7.19 | -0.169 |
| 13 | 81.2 | 80.1 | 80.1 | -1.09 | -1.12 | -0.0261 |
| 14 | -10.4 | -22.4 | -22.7 | -12.0 | -12.3 | -0.291 |
| 33 | 279.8 | 282.9 | 283.0 | 3.13 | 3.21 | 0.0750 |
| 44 | 96.8 | 116.4 | 116.9 | 19.6 | 20.1 | 0.472 |
| 66 | 92.9 | 100.3 | 100.5 | 7.40 | 7.58 | 0.178 |

Units: 10^9 N/m².

TABLE 10. ELASTIC COMPLIANCES.

| | sE | sD | sP | del sED | del sEP | del sDP |
|----|--------|--------|--------|---------|---------|----------|
| 11 | 4.93 | 4.79 | 4.78 | 0.143 | 0.146 | 0.00283 |
| 12 | -0.518 | -0.424 | -0.422 | -0.0945 | -0.0962 | -0.00169 |
| 13 | -1.28 | -1.24 | -1.23 | 0.0450 | -0.0461 | -0.00105 |
| 14 | 0.585 | 1.00 | 1.01 | -0.419 | -0.427 | -0.00798 |
| 33 | 4.32 | 4.23 | 4.23 | 0.0832 | 0.0852 | 0.00195 |
| 44 | 10.46 | 8.98 | 8.95 | 1.48 | 1.51 | 0.0282 |
| 66 | 10.90 | 10.42 | 10.41 | 0.475 | 0.484 | 0.00905 |

Units: 10^{-12} m²/N.

TABLE 11. PIEZOELECTRIC [e], [h], AND [a] VALUES.

| | e | h | a |
|----|-------|-------|-------|
| 15 | 2.72 | 7.21 | 7.39 |
| 22 | 1.67 | 4.43 | 4.54 |
| 31 | -0.38 | -1.00 | -1.03 |
| 33 | 1.09 | 2.88 | 2.94 |

Units: e: C / m²; h and a: 10^9 V/m.

TABLE 12. PIEZOELECTRIC [d], [g], AND [b] VALUES.

| | d | g | b |
|----|-------|-------|-------|
| 15 | 26.5 | 55.9 | 56.9 |
| 22 | 7.51 | 15.8 | 16.1 |
| 31 | -3.07 | -7.93 | -8.11 |
| 33 | 5.68 | 14.7 | 15.0 |

Units: d: 10^{-12} m / V; g and b: 10^{-3} m²/C.

TABLE 13. DIELECTRIC (eps) VALUES.

| | (eps)S | (eps)T | del (eps)TS |
|----|--------|--------|-------------|
| 11 | 377. | 474. | 97.1 |
| 33 | 247.0 | 254.6 | 8.52 |

Units: 10^{-12} F/m.

del (eps)TS = del (chi)TS

TABLE 14. DIELECTRIC (chi) VALUES.

| | (chi)S | (chi)T | del (chi)TS |
|----|--------|--------|-------------|
| 11 | 368. | 465.7 | 97.1 |
| 33 | 370. | 479. | 8.52 |

Units: 10^{-12} F/m.

del (chi)TS = del (eps)TS

TABLE 15. DIELECTRIC (bet) VALUES.

| | (bet)S | (bet)T | del (bet)TS |
|----|--------|--------|-------------|
| 11 | 2.65 | 2.11 | -0.543 |
| 33 | 2.64 | 2.58 | -0.0580 |

Units: 10^{-9} m/F.

TABLE 16. DIELECTRIC (zet) VALUES.

| | (zet)S | (zet)T | del (zet)TS |
|----|--------|--------|-------------|
| 11 | 2.72 | 2.15 | -0.567 |
| 33 | 2.70 | 2.64 | -0.0608 |

Units: $10^{(9)}$ m/F.

CONCLUSIONS

This report provides formulas interrelating the coefficients that appear in the several alternative sets of constitutive equations involving the elastic, piezoelectric, and dielectric properties of crystals. These are then specialized for crystals of class 3m; using measured values reported for lithium tantalate, numerical values of the elements of the polarization matrices are calculated.

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